

Derivation of continuum stochastic equations for discrete growth models

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We present a formalism to derive the stochastic differential equations (SDEs) for several solid-on-solid growth models. Our formalism begins with a mapping of the microscopic dynamics of growth models onto the particle systems with reactions and diffusion. We then write the master equations for these corresponding particle systems and find the SDEs for the particle densities. Finally, by connecting the particle densities with the growth heights, we derive the SDEs for the height variables. Applying this formalism to discrete growth models, we find the Edwards-Wilkinson equation for the symmetric body-centered solid-on-solid (BCSOS) model, the Kardar-Parisi-Zhang equation for the asymmetric BCSOS model and the generalized restricted solid-on-solid (RSOS) model, and the Villain-Lai-Das Sarma equation for the conserved RSOS model. In addition to the consistent forms of equations for growth models, we also obtain the coefficients associated with the SDEs.

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In recent years, the study of nonequilibrium surface growth has attracted considerable interest in both analytical and computational physics [1]. A number of discrete growth models and continuum stochastic equations have been proposed to describe the kinetic roughening properties of surface growth [2–7]. By studying these models and equations, we classify them into universality classes according to their scaling behavior and associate the continuum stochastic equations with the given discrete growth models.

In general, two methods have been widely used to establish the correspondence between a continuum growth equation and a discrete growth model. One method is to use Monte Carlo simulations to obtain the scaling exponents from the discrete model and compare them with those of the corresponding continuum equation. The other is to derive the continuum equation analytically from a given discrete model. Computational methodologies have contributed significantly to our understanding of epitaxial growth over the past few years and continue to do so unabated. Analytic derivations include methods using the principle of symmetry [8] or reparametrization invariance [9], and approaches starting from the master equation [10–13]. In particular, a systematic method proposed by Vvedensky *et al.* [10] has been successfully applied to the derivation of the continuum growth equations directly from the growth rules of the discrete model for several solid-on-solid discrete models [11–13]. The derivation procedure of Vvedensky *et al.* consists of two steps. First, the discrete stochastic equation is derived for the discrete growth model beginning with the master-equation description of the microscopic dynamics of the discrete model. Second, the discrete equation is transformed into a continuous stochastic equation via regularization by expanding the nonanalytic quantities and replacing them with analytic quantities. In this regularization procedure, the step function is approximated by an analytic shifted hyperbolic tangent function, which is expanded in a Taylor series. As pointed out by Předota and Kotrla [12], the choice of regularization scheme for the step function is ambiguous. Thus, the coefficients in the derived continuum stochastic equation cannot be determined uniquely.

In this Rapid Communication, we present a method for deriving the continuum stochastic equations from the discrete growth models. Our method can be applied to most of the models that are accessible via the method of Vvedensky *et al.* In addition to the derivation of stochastic equations consistent with the numerical solutions for the discrete models, our method predicts the coefficients in the stochastic equations. Our method begins with mapping of the discrete models onto reaction-diffusion systems with hard-core particles and sets up the master equation of the microscopic dynamics in the form of the Schrödinger equation. Next, borrowing the method introduced in Ref. [14], we derive the corresponding Fokker-Planck equation, and then the stochastic differential equation is obtained. We apply our method to three discrete growth models: the body-centered solid-on-solid (BCSOS) model, the generalized restricted solid-on-solid (RSOS) model, and the conserved RSOS (CRSOS) model.

The BCSOS model is one of the simplest microscopic growth models. Consider a surface built from square bricks rotated by $\pi/4$, without defects such as overhangs and vacancies. Each bond i contains a step $S_i = \pm 1$. The growth dynamics is as follows: Choose one of the columns at random. If this column is at the bottom of a local valley ($S_{i-1} = -1$ and $S_i = +1$), a particle adsorbs with probability p (and nothing happens with probability $1 - p$). If it is at the top of a local hill ($S_{i-1} = +1$ and $S_i = -1$), a particle desorbs with probability q (and nothing happens with probability $1 - q$). If it is part of a local slope ($S_{i-1} = S_i$), nothing happens. This model can be mapped onto the problem of the asymmetric exclusion process (ASEP). The process describes particles that hop independently with

hard-core exclusion along a one-dimensional lattice with a bias that mimics an external driving force. By denoting the descending slope as the particle (A) and the ascending slope as the vacancy(\emptyset), the microscopic growth dynamics can be mapped to a stochastic dynamical rule of the ASEP: the only transitions allowed for the site with neighboring bonds ($i-1, i$) are

$$\begin{aligned} A\emptyset &\rightarrow \emptyset A \quad \text{with probability } p, \\ \emptyset A &\rightarrow A\emptyset \quad \text{with probability } q. \end{aligned} \tag{1}$$

This model has been studied extensively in the literature by Monte Carlo simulations [15] and more recently it was realized that it can be solved exactly [16]. Furthermore, Derrida and Mallick calculated the diffusion constant associated with fluctuations of the current in the limit of $p \simeq q$ and derived the corresponding continuum stochastic equation with the coefficients correct up to the lowest order [17]. Krug *et al.* found the coefficients for the totally asymmetric, that is, $q = 0$, case [18]. Here, we apply our method to the ASEP to derive the corresponding stochastic equation. For simplicity, we set $p = 1$ and $q = x$ ($0 \leq x \leq 1$). For $x = 1$ the system is symmetric, whereas for $x = 0$ it reduces to the totally asymmetric case [19].

Introducing the annihilation and creation operators (\hat{a}_i 's and \hat{a}_i^\dagger 's, respectively) satisfying the mixed commutation relations explained in Ref. [14] and defining the state vector $|\psi; t\rangle \equiv \sum_C P(C; t)|C\rangle$, the master equation can be written as a Schrödinger-like equation:

$$\frac{\partial}{\partial t} |\psi; t\rangle = -\hat{H} |\psi; t\rangle, \tag{2}$$

where $P(C; t)$ is the probability for the system to be in a given microscopic configuration C at time t , and \hat{H} , called the Hamiltonian, is an evolution operator expressed in terms of \hat{a}_i 's and \hat{a}_i^\dagger 's. From now on, any operator will have a caret (e.g., \hat{a}, \hat{b}) and any symbol without a caret should not be confused with an operator. Occasionally, the same symbol is used to represent an operator and a density (e.g., \hat{a}_i and a_i). The Hamiltonian generating the time evolution of the BCSOS model is found to be

$$\hat{H} = - \sum_i \left(\hat{a}_i \hat{a}_{i+1}^\dagger + x \hat{a}_i^\dagger \hat{a}_{i+1} \right). \tag{3}$$

Since the diagonal terms that make \hat{H} stochastic have no role in our formalism, for simplicity, we omit these terms here and throughout this Rapid Communication. By involving the commutation relations between the Hamiltonian and some relevant operators such as $\hat{a}_i^\dagger \hat{a}_i$ and $\hat{a}_i^\dagger \hat{a}_i \hat{a}_j^\dagger \hat{a}_j$, and using the property of the projection state $\langle \cdot | (\hat{a}_i^\dagger + \hat{a}_i) = \langle \cdot |$ [14], where $\langle \cdot | \equiv \sum_C \langle C |$, we find the Kramers-Moyal coefficients [20] corresponding to the above Hamiltonian:

$$C_i = a_{i+1} + a_{i-1} - 2a_i - (1-x)[a_{i+1}(1-a_i) - a_i(1-a_{i-1})], \tag{4}$$

$$\begin{aligned} C_{ij} = & -[a_i + xa_{i+1} - (1-x)a_i a_{i+1}] (\delta_{i+1,j} - \delta_{ij}) \\ & + [a_{i-1} + xa_i - (1-x)a_i a_{i-1}] (\delta_{i,j} - \delta_{i-1,j}). \end{aligned} \tag{5}$$

Notice the absence of the caret on the a 's. From the coefficients C_i and C_{ij} , we write down the discrete stochastic equation

$$\frac{\partial a_i}{\partial t} = C_i + \xi_i, \tag{6}$$

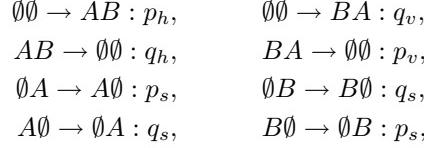
where a_i is the local density of the particle at i and $\langle \xi_i(t)\xi_j(t') \rangle = C_{ij}\delta(t-t')$. Replacing a_i by $(1-\nabla h)/2$ and taking the continuum limit, we obtain the continuum stochastic equation for the height variable h for the BCSOS model (and equivalently for the ASEP):

$$\frac{\partial h}{\partial t} = \frac{1-x}{2} + \frac{1+x}{2} \nabla^2 h - \frac{1-x}{2} (\nabla h)^2 + \xi(r; t), \tag{7}$$

with $\langle \xi(r; t)\xi(r'; t') \rangle = 4(1+x)\rho(1-\rho)\delta(r-r')\delta(t-t')$ (ρ is the stationary-state density, which is the same as the initial density). For the symmetric process ($x = 1$), the corresponding equation is the EW equation, whereas for the asymmetric process ($x \neq 1$) it is the KPZ equation. (Compare the coefficients with those in Refs. [17,18].)

Next we apply our method to the generalized RSOS growth model that was introduced by Neergaard and den Nijs [21]. They studied this model using an elegant mean-field type approach and derived the deterministic part of the KPZ equation. Our method is able to produce the stochastic (noise) part of the KPZ equation as well as the

same deterministic part as the method of Neergaard and den Nijs. The RSOS growth model describes the growth of simple cubic surfaces in which only monatomic steps are allowed. The heights at the nearest-neighbor columns can differ by only $\Delta h = 0, \pm 1$ (the RSOS constraint). After choosing one of the columns at random, one particle can be deposited at the site $i + 1/2$ with a probability 1 according to the height differences at i and $i + 1$. Employing the same parameter as in Ref. [21], we map this model onto the two-species hard-core particle system with the following processes:



where a particle A (B) stands for the ascending (descending) bond and a vacuum \emptyset represents the flat bond. The corresponding Hamiltonian is found to be

$$\hat{H} = - \sum_i \left[p_h \hat{a}_i^\dagger \hat{b}_{i+1}^\dagger + q_v \hat{b}_i^\dagger \hat{a}_{i+1}^\dagger + q_h \hat{a}_i \hat{b}_{i+1} + p_v \hat{b}_i \hat{a}_{i+1} \right. \\ \left. + p_s \hat{a}_i^\dagger \hat{a}_{i+1} + q_s \hat{a}_i \hat{a}_{i+1}^\dagger + q_s \hat{b}_i^\dagger \hat{b}_{i+1} + p_s \hat{b}_i \hat{b}_{i+1}^\dagger \right]. \quad (8)$$

Following the same steps as above, we obtain the Kramers-Moyal coefficients C_i^α and $C_{ij}^{\alpha\beta}$ (α, β indicate either A or B) as follows :

$$C_i^A = \frac{p_h + q_v}{2} v_i (v_{i+1} + v_{i-1}) + \frac{p_h - q_v}{2} v_i (v_{i+1} - v_{i-1}) - q_h a_i b_{i+1} - p_v b_{i-1} a_i \\ + \frac{p_s + q_s}{2} [a_{i+1} + a_{i-1} - 2a_i + a_i(b_{i+1} + b_{i-1}) - b_i(a_{i+1} + a_{i-1})] \\ + \frac{p_s - q_s}{2} [(a_{i+1} - a_{i-1})(1 - 2a_i) - (a_{i+1} - a_{i-1})b_i - a_i(b_{i+1} - b_{i-1})], \quad (9)$$

$$C_{ij}^{AA} = \left\{ \frac{p_h + q_v}{2} v_i (v_{i+1} + v_{i-1}) + \frac{p_h - q_v}{2} v_i (v_{i+1} - v_{i-1}) + q_h a_i b_{i+1} + p_v b_{i-1} a_i \right. \\ \left. + \frac{p_s + q_s}{2} [v_i(a_{i+1} + a_{i-1}) + a_i(v_{i+1} + v_{i-1})] \right. \\ \left. + \frac{p_s - q_s}{2} [v_i(a_{i+1} - a_{i-1}) + a_i(v_{i-1} - v_{i+1})] \right\} \delta_{ij} \\ - \{p_s(1 - a_i - b_i)a_{i+1} + q_s a_i(1 - a_{i+1} - b_{i+1})\} \delta_{i+1,j} \\ - \{q_s(1 - a_i - b_i)a_{i-1} + p_s a_i(1 - a_{i-1} - b_{i-1})\} \delta_{i-1,j}, \quad (10)$$

$$C_{ij}^{AB} = C_{ji}^{BA} = \delta_{i+1,j} (p_h v_i v_{i+1} + q_h a_i b_{i+1}) + \delta_{i-1,j} (q_v v_i v_{i-1} + p_v a_i b_{i-1}), \quad (11)$$

where $v_i = 1 - a_i - b_i$ and C_i^B (C_{ij}^{BB}) is obtained by the exchange $a \leftrightarrow b$ followed by $i + k \leftrightarrow i - k$ in C_i^A (C_{ij}^{AA}). By introducing the local slope $D \equiv a - b$ and the step density $S \equiv a + b$, we derive the deterministic parts of the stochastic equations for these two parameters:

$$\frac{\partial D}{\partial t} = \nabla \left[f_q (1 - S)^2 + s_d (1 - S)S + \frac{1}{4} h_g (S^2 - D^2) \right] \\ + \frac{1}{2} s_m \nabla^2 D + \frac{1}{4} (2s_m - a_s) \nabla [D \nabla S - S \nabla D], \quad (12)$$

$$\frac{\partial S}{\partial t} = 2c_s (1 - S)^2 - \frac{1}{2} a_s (S^2 - D^2) + s_d \nabla [(1 - S)D] \\ + \frac{1}{2} h_g [D \nabla S - S \nabla D] - c_s (1 - S) \nabla^2 S \\ + \frac{1}{2} s_m \nabla^2 S - \frac{1}{4} a_s [S \nabla^2 S - D \nabla^2 D], \quad (13)$$

where we have used the same notation for the parameters as in Ref. [21]; $c_s = p_h + q_v$, $a_s = p_v + q_h$, $s_m = p_s + q_s$, $f_g = p_h - q_v$, $h_g = p_v - q_h$, and $s_d = p_s - q_s$. The equation for the step density S is the same as that of Neergaard

and den Nijs. As pointed out in Ref. [21], the equation for the step density contains a mass term and the step density reaches its stationary value $S_0 = \left[1 + \sqrt{a_s/(4c_s)}\right]^{-1}$ after a characteristic time $\tau_s = (2\sqrt{a_s c_s})^{-1}$. Thus, although there are two order parameters, only the local slope fluctuates at time scales larger than τ_s . At larger time scales, the step density does not behave as an independent dynamic variable. It follows local fluctuations in the slope of the surface:

$$S = S_0 + \frac{1}{2}\tau_s a_s D^2 + \tau_s \left[s_d(1 - S_0) - \frac{1}{2}h_g S_0 \right] \nabla D + \dots \quad (14)$$

Substituting Eq. (14) for S and identifying $D = \nabla h$, the equation for the height variable becomes

$$\frac{\partial h}{\partial t} = v_\infty + \nu \nabla^2 h + \frac{\lambda}{2}(\nabla h)^2 + \xi, \quad (15)$$

where

$$\begin{aligned} v_\infty &= f_g(1 - S_0)^2 + s_d(1 - S_0)S_0 + \frac{1}{4}h_g S_0^2, \\ \nu &= \frac{1}{4}\tau_s[2s_d(1 - S_0) - h_g S_0][h_g S_0 - 4f_g(1 - S_0) + 2s_d(1 - 2S_0)] + \frac{1}{2}s_m(1 - S_0) + \frac{1}{4}a_s S_0, \\ \lambda &= -\frac{1}{2}h_g + \frac{1}{2}\tau_s a_s[h_g S_0 - 4f_g(1 - S_0) + 2s_d(1 - 2S_0)], \end{aligned} \quad (16)$$

and $\langle \xi(x, t)\xi(x', t') \rangle = D_{\xi\xi}\delta(x - x')\delta(t - t')$ with $D_{\xi\xi} = c_s(1 - S_0)^2 + s_m S_0(1 - S_0) + a_s S_0^2/4$. This equation is the KPZ equation corresponding to the general RSOS model. To compare these coefficients with numerical work, let us consider the simple RSOS model introduced by Kim and Kosterlitz (KK model) [4]. The KK model corresponds to $p_h = p_v = p_s = 1$ and $q_h = q_v = q_s = 0$. We obtain the corresponding coefficients $v_\infty = 4/9$, $A \equiv D_{\xi\xi}/(2\nu) = 2/3$, $\lambda = -5/6$. These values are consistent with the estimated values from a numerical study by Krug *et al.* [18].

Recently, a different growth model with a RSOS condition has been proposed and studied by Kim *et al.* [6,7]. Instead of rejecting the particle when the RSOS condition is not satisfied, this model allows the deposited particle to hop to the nearest site where the RSOS condition is satisfied. Thus, this model has the constraint of a conserved growth condition and is called the conserved RSOS model. The detailed derivation of Villain–Lai–Das Sarma (VLD) equation from the CRSOS model will be published elsewhere [22]. Here we only sketch the procedure and report the result. The procedure is similar to the one used to get the KPZ equation from the RSOS model except for some complicated calculation. After some algebra, we find the VLD equation

$$\frac{\partial h}{\partial t} = -\tilde{\nu} \nabla^4 h + \tilde{\lambda} \nabla^2 (\nabla h)^2 + \eta, \quad (17)$$

where $\tilde{\nu} = (21 - 12\sqrt{2})/2$, $\tilde{\lambda} = (10 - 3\sqrt{2})/2$, and $\langle \eta(x, t)\eta(x', t') \rangle = D_{\eta\eta}\delta(x - x')\delta(t - t')$ with $D_{\eta\eta} = (2\sqrt{2} - 1)/2$. In deriving the above equation, we kept only the most relevant terms, and found that neither the EW nor the KPZ term exists in the growth equation. It is known, however, that higher order terms of the form $\nabla(\nabla h)^{2n+1}$ ($n \geq 1$) generate the EW term by the dynamic renormalization group [23]. Hence we should investigate the possibility of occurrence of these terms. Indeed, we found that the dangerous term of the form $\nabla(\nabla h)^{2n+1}$ does not arise in the derivation of the VLD equation [22]. Consequently, we concluded that the continuum equation of the CRSOS model is the VLD equation.

Although the VLD equation was derived by Huang and Gu [13] using the master-equation description with the regularization procedure proposed by Vvedensky *et al.*, there were some ambiguities in choosing the regularization of the step function and thus the coefficients could not be predicted, whereas, in our derivation, we are able to predict the coefficients for the VLD equation corresponding to the CRSOS model. Unfortunately, however, there is no numerical method, to our knowledge, to find $\tilde{\nu}$ and $\tilde{\lambda}$ for a microscopic model. Numerical studies up to now can argue only that $\tilde{\lambda}$ may be positive [7], which is consistent with our derivation.

In deriving the VLD equation, we recognized the interesting aspect of the RSOS model. When we allow hopping processes only up to distance l_0 , the stochastic equation for the height variable eventually becomes the KPZ one [22]. This is contradictory to previously reported simulation results [24]. Kim and Yook studied the RSOS model with finite-distance hopping by Monte Carlo simulation and concluded that there is a phase transition at finite l_0 from the KPZ class ($l_0 = 0$) to the VLD class ($l_0 = \infty$). However, this conclusion seems to be a finite-size effect. In fact, we have confirmed our argument by carrying out a Monte Carlo simulation with sufficiently large system size for several l_0 [22].

In summary, we have presented a formalism for deriving the continuum stochastic differential equations corresponding to discrete growth models. Applying the formalism to the BCSOS model, we derived the EW equation for the symmetric process and the KPZ equation with exact coefficients for the asymmetric process. The RSOS model was also studied with the general probabilities for possible processes. We derived the KPZ equation with a fluctuating noise part as well as the deterministic part, which is the same as the result of Neergaard and den Nijs. For the special case with $p = 1$ and $q = 0$ (the KK model), our coefficients are consistent with the numerical results of Krug *et al.* [18]. Finally, we applied our formalism to the conserved RSOS model. For the CRSOS model, we found that the VLD equation is the corresponding continuum SDE. However, if we allow only finite hopping ($l_0 < \infty$), the system belongs to the KPZ class eventually. We also predict the coefficients of the VLD equation for the CRSOS model.

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